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Determination of the elastic constants of zinc single crystals from diffuse X-ray scattering*

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The elastic constants of single crystals of zinc have been studied using diffuse X-ray scattering. Reciprocal nodes 004 and 200 were involved in the study. A microphotometer survey of the diffuse reflections gave intensity for a number of directions in reciprocal space. From the intensities the elastic ratios were evaluated and finally the absolute values determined using the compressibility data for zinc. The values in units of 10^{11} dynes. cm^{-2} are : $c_{11} = 16{\cdot}97$, $c_{12} = 2{\cdot}72$, $c_{13} = 5{\cdot}62$, $c_{33} = 7{\cdot}35$, $c_{44} = 4{\cdot}56$ and $c_{66} = 7{\cdot}12$. Results are comparable to the values of elastic constants determined by various other techniques.

1. Introduction

Crystal dynamics has been successfully dealt using the phenomena of diffuse X-ray scattering. Its study began as a means of accounting for the dependence of the intensity of normal Bragg-Laue reflections on temperature. This led to the theory of the connection with the elastic properties of crystals and of the force constants between the constituent atoms. A large number of authors have made determinations of elastic spectrum studying thermal diffuse scattering of X-rays. A full review to it is by Wooster (1962). Lastly diffuse reflection studies have been applied to molecular crystals (Joshi & Kashyap 1964; Chandra & Hemkar 1973). In studying the elastic constants of metal crystals with cubic structures method of diffuse reflection was applied with great success, but no attempt was made with the crystals having a lower symmetry so far. To test the applicability of the method elastic properties of hexagonal zinc metal crystals were undertaken. The photographic technique of recording diffuse X-ray reflection was employed since it is simple, practicable and do not requires the stabilization of the X-ray output. From the single crystal diffuse reflection photographs elastic ratios were determined.

* This work is dedicated to the memory of Late Professor Kedareshwar Banerji.

2. Theory

Thermal diffuse scattering resulting out of thermal motions which have their close relations with the elastic constants of the atoms is simply the sum of contributions from multi-phonon scattering interactions. The rel-vector H^* defines the diffuse reflection intensity from Wooster (1962) as

$$I(H^*) = |f_T|^2 \frac{KT^2}{\tau} \frac{H^{*2}}{K^{*2}} K[f]_G \qquad \ldots (1)$$

where $K[f]_G$ represents the *K-surface* which is defined as

$$K[f]_G = G_i G_k [A^{-1}]_{ik}$$

where f corresponds to the direction cosines f_1, f_2, f_3 of the wave normal to the elastic wave (rekha) and G represents the direction cosines G_1, G_2, G_3 of the line joining the nearest relp to the origin (rel-vector). By studying diffuse scattering intensity about suitable relps all the values of the constants are obtained using relation for cubic compressibility and elastic modulii for hexagonal zinc as

$$\beta = \frac{1}{C_{11}}\left\{2 + \frac{1}{\chi_{33}} + \frac{4}{\chi_{13}} + \frac{2}{\chi_{12}}\right\} \qquad \ldots (2)$$

where χ_{12}, χ_{13} and χ_{33} are the elastic ratios.

3. Experimental

Hexagonal zinc-metal single crystals belonging to $D_{6h}{}^4$ crystal class were grown by Bridgemann's technique. The method consists in lowering a self designed tube of pyrex glass containing molten pure (99·9%) zinc through a vertical furnace. The tube was allowed to creep through the furnace at a uniform rate of 8 mm/hour. The tube was so fabricated that its bottom formed a hooked capillary. This is essential to induce a single crystalline growth. The tube after it reached the bottom, was allowed to cool for another 24 hours and then brought out and broken open. After removal from the glass tube the crystal was etched in a solution consisting hydrogen peroxide (3 parts), glacial acetic acid (2 parts) and water (1 part). Usually the whole block was a single crystal but when it was not so, there appears boundaries between separate crystals, which were easily revealed by simple etching for a few minutes. The crystals were then tested for being single. Its orientations were determined by X-ray photographs using Cu K$_\alpha$ radiation and faces parallel to the required crystallographic planes cut with a microtome and electropolished.

The crystals were mounted on Unicam oscillation goniometers with the plane of $(h00)$ and $(00l)$ faces vertical. The radiation used was Cu K$_\alpha$ with a balanced filter (Ni-Co) and the tube run at 15 KV and 20 mA. This eliminates higher harmonics.

The distribution of intensity over the diffuse spots were scanned with a self-recording Moll Microphotometer. Contour maps of the respective diffuse spots were constructed from the computed values of intensities obtained from the ordinates of the photometric curve by comparision with the calibration wedge, following the method of Robinson (1933) The value of intensity corresponding to each rekha was obtained from the experimental contours of the diffuse spots. Measured intensities were corrected for divergence due to finite size of the laue spot. Correction due to general scattering was determined from the graph of intensity vs $1/K^{*2}$ as given in figures 1 and 2. Preliminary values of the stiffness constants were next calculated. These values were used in the calculation of second order contribution which was required to be subtracted from the diffuse scattering intensity measured.

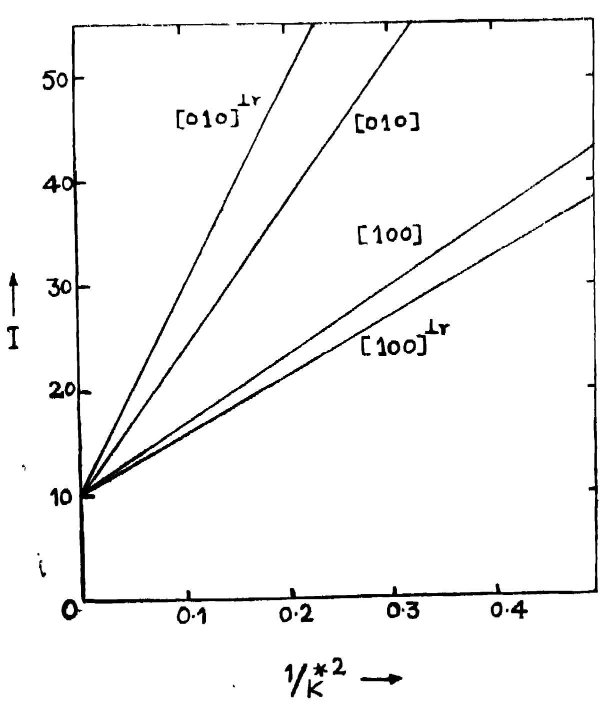

Fig. 1. Curves showing the variation of diffuse intensity plotted as function of $1/K^{*2}$ for zinc single crystals using the relp 004 and various rekhas.

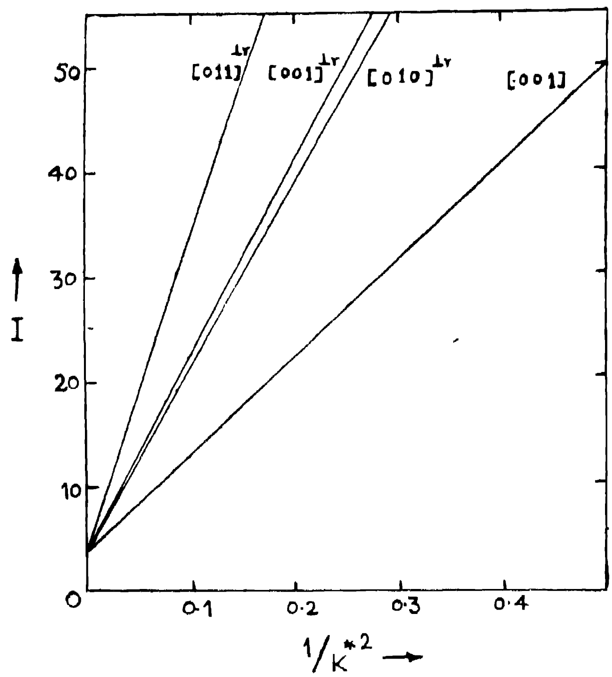

Fig. 2. Curves showing the variation of diffuse intensity plotted as function of $1/K^{*2}$ for zinc single crystals using the relp 200 and various rekhas.

4. Results

The reciprocal lattice points used for the evaluation of the elastic constants are 004 and 200 using $h00$ and $00l$ faces of Zinc single crystals. Firstly we aim at the ratios of the elastic constants which were contained in the relative values of diffuse scattering corresponding to different rekhas. From eq. (1) the intensity of diffuse X-rays is inversely proportional to K^{*2}. Hence the ratio of elastic constants were obtained (table 1) from the slope of I vs $1/K^{*2}$ graphs as in figures 1 and 2. The absolute values of elastic constant were obtained utilizing the expression for the value of compressibility for zinc which depends on the absolute value of one or more of the elastic constants from eq. (2). By utilizing $\chi_{66} = (1 - \chi_{12})$ for hexagonal crystal, the value of χ_{1v} was calculated to be 0·16. The determined values of elastic constants are given in table 2. Results obtained are comparable to the reported values by Waterman (1958) and values given in Solid State Physics (1958)

Table 1

$$\frac{K[100]_{h00}}{K[010]_{h00}} = \frac{c_{66}}{c_{11}} = 0{\cdot}42$$

$$\frac{K[001]_{001}}{K[010]_{001}} = \frac{c_{44}}{c_{33}} = 0{\cdot}62$$

$$\frac{K[100]^{1}r_{h00}}{K[010]^{1}r_{h00}} = \frac{c_{44}}{c_{11}} = 0{\cdot}27$$

$$K[001]^{1}r_{001} = \frac{c_{03}}{c_{33}} = 0{\cdot}73$$

Table 2

Elastic Constants	Calculated value in units of 10^{11} dyne/cm^2	Reported values in 10^{11} dyne/cm^2
C_{11}	16·97	16·10
C_{12}	2 72	3·25
C_{13}	5·62	5·01
C_{33}	7·35	6·10
C_{44}	4·56	3·83
C_{66}	7·12	6·83

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